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NUMERICAL SOLUTION OF THE PROBLEM OF SCATTERING ON A CLASS OF SINGULAR POTENTIALS

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NUMERICAL SOLUTION OF THE PROBLEM OF SCATTERING ON A CLASS OF SINGULAR POTENTIALS

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ABSTRACT

Method and main results of the numerical integration of the differential equations for the non-relativistic scattering on some singular potentials of the singularity r^{-4} are presented. Thereby a clear-cut decision was obtained as to the validity of the available analytical approximations for high energies.

РЕЗЮМЕ

При рассеянии на сингулярных потенциалах различные аналитические приближения для предела фазы рассеяния при высоких энергиях дают различные результаты. В настоящей работе мы пытались с помощью численных расчетов исследовать нерелятивистское рассеяние на потенциале с сингулярностью типа r^{-4}.

KIVONAT

Bemutatjuk az r^{-4} tipusu szingularitást mutató potenciálokon történő szóródás problémájának numerikus megoldását nem relativisztikus tárgyalásban. Sikerült ilymódon eldönteni, melyik ismert analitikus közelités adja a legjobb eredményt a nagyenergiák határesetében.

Method of and the main results obtained in the numerical integration of the differential equations for the non-relativistic scattering on some singular potentials of the type $V(r) = g^2 r^{-4}$ are presented.

Repulsive singular potentials that diverge more rapidly than r^{-2} at $r = o$ are considered to be physically interpretable owing to the existence of a unique regular scattering solution. Application involves simulation of the soft core in the interaction between nucleons as well as that of the repulsive shortrange contribution to the intermolecular forces. Further, the effective potentials in non-renormalizable field theories were also found singular.

Effect of the singularity at the origin manifests itself most clearly in the high-energy scattering. In particular, the phase shift $\delta_\ell(k)$ does not converge, in contrast to the phase shift of regular problems, to a finite constant as the wave number $\underline{k}$ goes to infinity. According to various analytical approximations [1-4] the asymptotical behaviour of the phase shift for the potential $V(r) = g^2 r^{-m}$ is dominated by the term

$$\delta_\ell(k) \underset{k\to\infty}{\sim} - A_o\, g^{2/m}\, k^{1-2/m} \quad . \qquad /1/$$

While the $\underline{g}$- and $\underline{k}$-dependence is common in all these approaches, the coefficient $\underline{A_o}$ has different numerical values in each calculation. E.g. for the case $\underline{m} = 4$ Jabbur [1] found $\underline{A_o} = 1.1667$ by an approximation to the WKB-method. Bertocchi et al. [2] as well as Paliov and Rosendorff [3] obtained $\underline{A_o} = 1.1977$ in explicit WKB-calculation. Finally, the variable phase approach, developped by Calogero [4], lead to $\underline{A_o} = 1.1811$. According to a critical review of Frank et al. [5] the value $\underline{A_o} = 1.1977$ should be exact if the WKB-method in refs. [2,3] constitutes actually asymptotical expansions.

Now, we briefly report on a recent numerical investigation of the scattering on the energy-dependent potential

$$\begin{aligned} V(r) &= g_o^2\, e^{-\mu r_t(k)} r^{-4} \equiv g^2\, r^{-4}, \quad && r \leq r_t(k), \\ &= g_o^2\, e^{-\mu r} \quad r^{-4} \quad , && r > r_t(k) \end{aligned} \qquad /2/$$

where $r_t(k) = (g_o/k)^{1/2}$ gives the classical turning point of the problem without the exponential cut-off ($\mu = o$). The long-range cut-off in eq. /2/ does not influence the high-energy behaviour of the scattering. For large distances $r > r_t(k)$ the phase-equation [6] for the S-waves

$$\frac{d\delta_o(k,r)}{dr} = -k^{-1} V(r) \quad \{\sin [kr + \delta_o(k,r)]\}^2 \qquad /3/$$

was integrated where $\delta_o(k,r)$ is the phase function, i.e. the phase shift for the potential $V(r')$ cut off at $r' = r$. For $r < r_t(k)$, however, the Schroedinger equation was dealt with. Integration started from $r = r_o(k) < r_t(k)$ defined by

$$k^2 \{V(r_o)\}^{-1} = \varepsilon \qquad /4/$$

where the fitting parameter ε was chosen in practice in the region $\varepsilon = 10^{-5}-10^{-3}$. Below such an $r_o(k)$ the influence of the energy k^2 on the wave function was considered to be negligible. The physical wave function $u_o(k,r)$ was fitted smoothly at $r = r_o(k)$ to the zero-energy regular solution which is known to be exactly

$$u_o(k=o, r) = r\, e^{-g/r} . \qquad /5/$$

The smaller is ε the smaller becomes the <u>fitting error</u> Δ_f caused by the inexactness of the boundary conditions. As to the <u>truncation error</u> of the corrected Runge-Kutta procedure [7], the leading term in the one-step relative error of $f(k,r) = u_o'(k,r)/\, u_o(k,r)$ was found to be

$$\Delta_{RK}(r) \underset{r\to o}{\sim} \frac{1}{120} (g^2 r^{-4} - k^2)^3 \, h^5(r) \qquad /6/$$

where $h(r)$ is the integration step in the point r. To control this error one way is to keep it constant, $\Delta_{RK}(r) = \Delta$, and to work at $r \sim r_o$ with

$$h(r) \approx (120\Delta)^{1/5} \, g^{-6/5} \, r^{12/5} . \qquad /7/$$

Nevertheless, in the actual calculations we worked with $h(r) = \text{const.}\, r^3$. The RK-error as expressed in terms of the parameter ε from the eqs. /4/ and /6/ is for $r = r_o$ generally

$$\Delta_o \equiv \Delta_{RK}(r_o) = \frac{1}{120} k^6 \, \varepsilon^{-3} \, h^5(r_o). \qquad /8/$$

As $h(r)$ is fixed by the available computing time one has to find the optimum value for ε to get the minimum total error which includes both Δ_f

and Δ_{RK}. The estimated RK-errors at $r = r_o$ for each k are given in the last column of Table 1. The round-off error seems to be negligible in

Table 1

S-wave phase shifts and a_o (k,g) for the potential /2/ from the numerical integration. For comparison also values of A_o from analytical approaches are included

k	g_o	$\log\varepsilon$	$\log h_o$	β	$\delta_o(k)$	$a_o(k,g)$	$\log \Delta_o$
50	1.0	-3.0	-6.0	0.1	-7.3580	1.1931	-13.0
100	1.0	-3.0	-5.7	0.1	-10.8492	1.1929	- 9.5
200	1.0	-3.0	-5.6	0.1	-15.7989	1.1936	-7.2
1000	1.0	-3.0	-5.3	0.1	-36.7256	1.1956	-1.5
	1.0	-3.0	-5.3	1.0	-36.7287	1.1957	-1.5
	1.0	-4.0	-6.7	0.1	-36.7256	1.1956	-5.5
	1.0	-5.0	-7.0	0.1	-36.7062	1.1950	-4.0
	5.0	-4.0	-6.7	0.1	-82.0178	1.1919	-6.5
	10.0	-4.0	-6.2	0.1	-115.2179	1.1894	-3.1
5000	5.0	-4.0	-6.3	0.1	-186.7199	1.1953	+4.5
10000	0.1	-4.0	-8.7	0.5	-37.0719	1.1981	+10.5
	0.4	-4.0	-7.7	0.5	-83.7446	1.1975	-4.5
	1.0	-3.0	-6.7	0.2	-118.4461	1.1957	-2.5
	1.0	-4.0	-7.2	0.2	-118.6357	1.1972	-2.1
	5.0	-4.0	-6.2	0.2	-265.1352	1.1959	-3.3
	10.0	-4.0	-5.7	0.2	-374.0369	1.1947	+5.5
30000	1.0	-3.0	-6.5	0.3	-206.5187	1.1976	+1.3
	5.0	-4.0	-6.0	0.3	-461.2010	1.1967	+1.8
	1.0	-4.0	-7.0	0.3	-206.3475	1.1976	+10.0

	A_o
Ref. [2,3]	1.1977
Ref. [4]	1.1811
Ref. [1]	1.1667

the 16-digit precision calculation that workes with a minimum step of the order $h_o = h(r_o) = 10^{-9}$. For the external region $r > r_t(k)$ the integration step was chosen r-independent and governed by the condition

$$k\,h(r) = \beta \qquad /9/$$

with the actual value of the constant β in the range 0.1-1.0. Calculations were carried out invariably with $\mu = 1.0$.

The phase equation and the differential equation for $f_o(k,r)$ were satisfied by the solution throughout the wave number range k = 50 - 30 000 units to at least 13 digits. Qualitative checks such as the monotonic decrease and early convergence of the phase function in terms of r - both depend on the integrated behaviour of the solution - worked also surprisingly well. Therefore, it was concluded that the effect on $f_o(k,r)$ or the unavoidable admixture of the irregular solution remained negligible also for the large values of r.

The phase shift $\delta_o(k)$ was obtained as the limiting value of the phase function for large r . The constant A_o of eq. /1/ was approached by

$$a_o(k,g) \triangleq \{ -\delta_o(k) + \frac{\pi}{4} \} g^{-1/2} k^{-1/2} \underset{k \to \infty}{\to} A_o . \qquad /10/$$

Extraction of the phase shift from the wave function in the lower r-region introduces a mod-π uncertainty which had to be removed by a comparison to the analytical approximations [1-4].

Main features of the results are summarized in Table 1. The obvious convergence of the series $a_o(k,g)$ justifies the asymptotical k-dependence of the phase shift as given by eq. /1/. Practical independence of $a_o(k,g)$ from $\underline{g}$ strongly supports the correctness of the g-dependence in the analytical approaches. In the particular case k = 10 000, $a_o(k,g)$ changed only 0.4 % while the coupling constant g^2 was increased by the factor 10^4. It is quite surprising that the $a_o(k,g)$ obtained in the case g = 10 excellently fits into the whole scheme in spite of the unacceptable large value of the estimated RK-error. The actual error for $r \sim r_o(k)$ must be well below the estimation given by eq. /8/. Also noteworthy is the stability of the calculated phase shift against variation of the parameters ε or β eg. for k = 1000. Data of Table 1. suggest that the WKB-calculations of refs. [2,3] should be regarded correct in the asymptotical region of the wave number. Results obtained for A_o by the WKB-approach are reproduced by $a_o(k,g)$ of the numerical method with a relative accuracy of 10^{-3} for k = 10 000 and of 10^{-4} for k = 30 000.

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